

Resistivity saturation revisited: results from a dynamical mean field theory

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We use the dynamical mean field method to study the high-temperature resistivity of electrons strongly coupled to phonons. The results reproduce the qualitative behavior of the temperature and disorder dependence of the resistivity of 'A-15' materials which is normally described in terms of saturation, but imply that the resistivity does not saturate. Rather, a change in temperature dependence occurs when the scattering becomes strong enough to cause a breakdown of the Migdal approximation. *PACS: 72.10-d, 72.10.Di, 72.80.Ga*

The conventional [1] theory of the temperature dependent resistivity of metals predicts that at temperatures greater than the phonon Debye frequency ω_D the resistivity, ρ , behaves as

$$\rho = A_\rho T + B_\rho \quad (1)$$

with the temperature coefficient A_ρ proportional to the electron-phonon coupling strength and residual resistivity B_ρ proportional to the impurity concentration. The theory accounts well for the properties of many metals but fails in a number of important cases. The first to attract widespread attention were the 'A-15' materials such as V_3Si and Nb_3Ge . In these compounds the electron-phonon coupling is unusually strong and although the high temperature $\rho(T)$ may be crudely fit to Eq. 1, A_ρ is much smaller than expected and, crucially, B_ρ is large even in pure samples [2]. Further, the effects of extra disorder (induced e.g. by radiation damage) are not additive: the extra disorder-induced resistivity is temperature dependent, being larger at lower T and smaller at higher T ; indeed for sufficiently high disorder levels $\rho(T)$ becomes flat and then $d\rho/dT$ becomes negative [3]. This complex of behaviors was named 'resistivity saturation' by Fisk and Webb [2]. Interest in this long-standing problem has been increased by observations that in a number of materials in which electron-electron interactions are believed to be important, including the high- T_c cuprates [4], the A_3C_{60} materials [5], and $SrRuO_3$ [6], $\rho(T)$ increases rapidly with increasing temperature and exhibits no signs of saturation even in the sense defined above, although the resistivity becomes much larger than that of A-15s. A recent paper [7] argued that this *absence of saturation* was itself anomalous and interesting.

Ref [2] has led to a large but still inconclusive literature on the cause of the phenomenon [8–11]. Eq 1 is the mathematical statement that ρ is proportional to lattice disorder, i.e. that electrons are scattered by displacements, due either to thermal fluctuations or defects in the crystal, of ions (labelled by i) from their ideal crystallographic positions. Its derivation is based

on three assumptions: (1) at temperatures greater than ω_D , the thermal fluctuations of the ions may be modelled in terms of classical harmonic oscillators with spring constant k ; equipartition then implies $\langle x_i^2 \rangle \sim T/k$ plus a T -independent term arising from defects, (2) the electron-ion interaction may be treated by second-order perturbation theory so that if the electron-ion coupling is g the electron scattering rate is $g^2 \langle x_i^2 \rangle$ and (3) usual Boltzmann transport theory may be used to relate the resistivity to the scattering rate. Combining these considerations yields Eq 1 with $A \sim g^2/k$ and B proportional to the impurity concentration.

Deviations from Eq 1 must come from the breakdown of one of the assumptions. Many authors have focussed on (3), however attempts to generate a systematic series of 'multiple scattering' corrections to the Boltzmann equation have produced a multiplicity of terms whose interpretation and range of validity have not been clear (see, e.g. [8]). However, examination of assumption (3) led Allen and Chakraborty to an important observation concerning the *magnitude* of the resistivity [8]. In the A-15 materials, the carriers are d-electrons and although the total carrier density is 4 d-electrons per metal ion, i.e. $n = 12$ per formula unit, the band structure is such that only one d-band crosses the fermi surface implying $n = 1$ per formula unit. The remaining d electrons are contained in filled bands which are very close to the fermi energy and to empty bands. A moderately large scattering rate will mix the full and empty bands with the conduction band, leading to a drastic increase in the effective number of carriers. Ref [8] concluded that while the effect does not fully explain the observed 'saturation' behavior, it does permit the magnitude of the high temperature resistivity to vary dramatically between different systems. We note here that the ruthenates and cuprates do not have many filled and empty d-bands near the fermi surface, and so may have a lower carrier density and thus higher resistivity than do the A-15s.

Belitz and Schirmacher [9] used a 'memory function' formalism to study a model of electrons interacting with

phonons via both density and stress couplings. In their model ρ increased indefinitely with T due to an interplay between scattering caused by the density coupling and hopping induced by the stress coupling. Our results suggest that the stress coupling and associated hopping are not necessary to reproduce the phenomenon.

Yu and Anderson [11] focussed instead on assumptions (1) and (2), arguing that a strong electron-phonon coupling could lead to a spontaneously generated double-well potential for the phonon, rendering the second-order perturbation theory treatment invalid and requiring a sophisticated quantum treatment. Our results support the idea that a strong electron-phonon coupling is the essence of the problem but imply that neither double-well formation nor quantum effects are essential.

In this Letter we calculate the resistivity of a model of electrons coupled with arbitrary strength to phonons. Because we seek to understand the fundamental mechanism underlying the saturation phenomenon we consider the simplest possible model: spinless electrons coupled to dispersionless phonons and to static disorder. Because saturation is a high- T phenomenon we further specialize to classical phonons ($\omega_D \rightarrow 0$). The Hamiltonian $H = H_{el} + H_{ph} + H_{el-ph} + H_{disorder}$ with electronic part $H_{el} = -\sum_p \epsilon_p d_p^\dagger d_p$ describing motion of electrons in a band with dispersion ϵ_p phonon part $H_{ph} = \sum_i \frac{1}{2} k x_i^2$, an electron-phonon coupling $H_{el-ph} = g \sum_i x_i (d_i^\dagger d_i - n)$, and an disorder part $H_{disorder} = \sum_i w_i (d_i^\dagger d_i - n)$. The form for $H_{disorder}$ corresponds to electrons scattered by random point defects which may be thought of as frozen-in lattice distortions of amplitude w_i/g . The mean density of electrons is n so $x = 0$ is the equilibrium phonon state for a uniform distribution of electrons. We assume the random site energies w_i associated with the disorder are distributed according to $P_{dis}(w) = \exp(-w^2/\eta^2)/(\sqrt{2\pi}\eta^2)$.

We define the parameter t to be one quarter of the full electron bandwidth; we measure all energies and temperatures in units of t . Rescaling the phonon coordinate $x \rightarrow x/\sqrt{k}$ shows that the dimensionless parameter describing the electron-phonon coupling is $\lambda = g^2/(kt)$ (this λ is a factor of π larger than the conventional MacMillan parameter). At low T the model may be solved by the usual Migdal perturbation theory, which is an expansion in $\lambda\sqrt{\max(\omega_D, T)/t}$ [12]. To treat arbitrary coupling strengths we employ the dynamical mean field approximation [13] which becomes *exact* in the limit of spatial dimensionality $d \rightarrow \infty$ and which comparisons to other techniques and to experiment have shown to be quantitatively accurate in $d = 3$. The approximation may be derived from the assumption that the electron Green function G is

$$G(\epsilon_p, i\omega_n) = [i\omega_n - \Sigma(i\omega_n) - \epsilon_p + \mu]^{-1}. \quad (2)$$

where the self-energy Σ is taken to be p -independent.

This ansatz implies that all interaction effects are derivable from the local (p -integrated) Green function, G_{loc} given by $G_{loc}(i\omega_n) = \int \frac{d^d p}{(2\pi)^d} G(\epsilon_p, i\omega_n) = \int \frac{d\epsilon_p \mathcal{D}(\epsilon_p)}{i\omega_n - \Sigma(i\omega_n) - \mu - \epsilon_p}$. G_{loc} is itself given in terms of a mean field function $a(\omega)$ determined by an equation which depends on the density of states \mathcal{D} ; we choose the semicircular form $\mathcal{D}_{semi}(\epsilon_p) = \sqrt{4t^2 - \epsilon_p^2}/(2\pi t^2)$, so that

$$a(\omega) = \omega + \mu - \int_{-\infty}^{\infty} dx dw \frac{P_{phonon}(x, w) P_{dis}(w)}{a(\omega) + gx + w} \quad (3)$$

with the phonon probability distribution

$$P_{phonon} = \frac{1}{Z_{loc}} \exp \left[-\frac{x^2}{2T} + \int d\omega \ln [a(\omega) + gx + w] \right] \quad (4)$$

with $Z_{loc} = \int dx dw P_{phonon}(x, w) P_{dis}(w)$. $G_{loc}(\omega) = \frac{\partial \ln Z_{loc}}{\partial a(\omega)}$ and $\Sigma(\omega) = a(\omega) - G_{loc}^{-1}(\omega)$. This treatment of static disorder is equivalent to the familiar coherent potential

We solve the equations numerically; computational details are given in ref [14]. The conductivity may be calculated from [13]

$$\sigma \simeq \int d\omega \int d\epsilon_p \mathcal{D}(\epsilon_p) [Im G(\epsilon_p, \omega)]^2 \cosh^{-2} \frac{\omega}{2T} \quad (5)$$

(Ref [13] takes the current operator to be independent of ϵ_p ; this does not affect results in any important way).

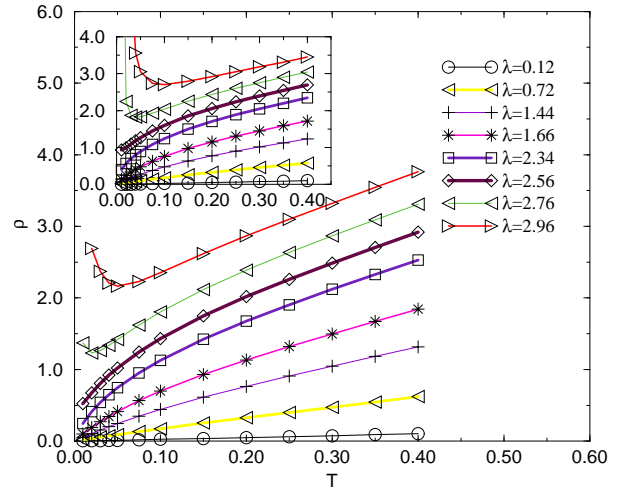


Fig 1 Resistivity $\rho(T)$ vs temperature T (in units of t =bandwidth/4) at various couplings λ for density $n=1/4$. Inset: Same couplings, density $n=1/2$.

Fig. 1 shows the calculated resistivity ρ vs. temperature T at various couplings (assuming $\eta = 0$ i.e. no disorder) for density $n=1/4$; the inset shows the same calculation for $n=1/2$. Clearly the two fillings display the same qualitative behavior: at weak coupling, the resistivity has the usual linear T -dependence with a zero

offset and a slope proportional to λ . (Quantum effects neglected here would cause the resistivity to drop dramatically once T is reduced below ω_D but do not affect [12] the behavior at $T > \omega_D$; our results are only meaningful for $T > \omega_D$). For the narrow bands typical of A-15 materials, $T = 0.1$ corresponds to a temperature of order 300K, and only the results for $T > 0.1$ should be regarded as physically meaningful. At intermediate coupling, the high-temperature resistivity displays the essential features of the 'saturation' behavior found in the data, namely an apparently linear T dependence with non-zero offset and slope rather weakly dependent on λ . At very strong coupling, the high- T behavior is not much changed (except that the offset becomes larger relative to the slope) but at low T the system becomes insulating ($d\rho/dT < 0$) below a λ -dependent characteristic temperature T_{gap} because a gap of size T_{gap} opens at low T in the electron spectral function. Our interest is in the high- T behavior; the low- T insulating regime is extensively discussed in Ref [14].

We now determine the origin of the saturation behavior. The first issue is the relation between the resistivity and the electron self-energy. Fig 2 plots the calculated resistivity versus the imaginary part of the electron self-energy evaluated at the fermi surface, ($\Sigma''(\omega = 0)$).

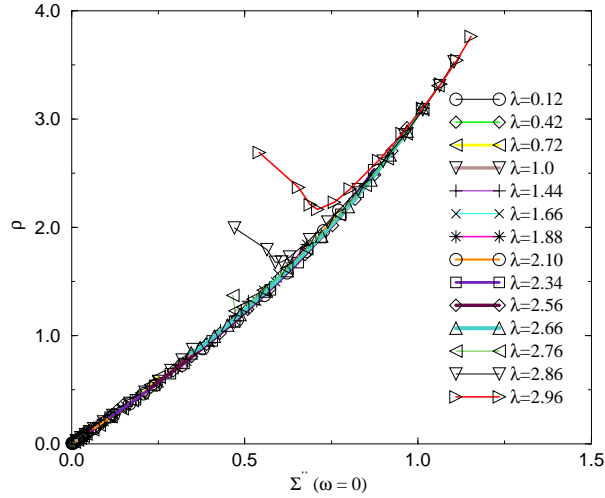


Fig 2 Resistivity ρ plotted against fermi surface scattering rate Σ'' (given in units of $t=\text{bandwidth}/4$) for various couplings, with temperature as an implicit parameter. The points which break away from the universal curve correspond to the low T insulating regime.

One sees that except in the insulating low- T strong coupling gapped regime, ρ is a *universal* function of $\Sigma''(0)$. At weak coupling, $\rho \sim \Sigma''(0)$ as expected; at stronger couplings ρ increases *faster* than $\Sigma''(0)$. Thus assumption (3) is not the issue.

We next consider phonon anharmonicity. Fig 3 shows the mean square displacement of the oscillator coordinate as a function of temperature for the coupling strengths

used in Fig. 1. At weak coupling one sees the classical behavior $\langle x^2 \rangle \sim T$ with zero intercept. As the coupling is increased the high- T behavior acquires the form $\langle x^2 \rangle \sim A_{\text{phonon}}T + B_{\text{phonon}}$. However, a comparison of Figs 1 and 3 shows the ratio $B_{\text{phonon}}/A_{\text{phonon}}$ is much less than the ratio B_ρ/A_ρ ; in other words, the resistivity curves are much flatter than the lattice displacement curves.

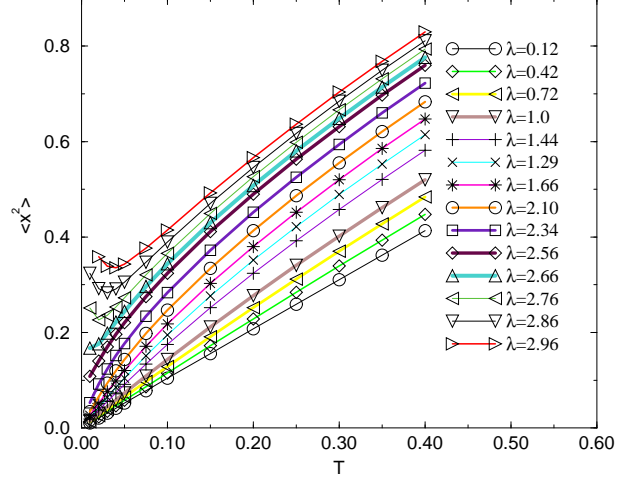


Fig 3 Mean square lattice displacement $\langle x^2 \rangle$ vs. temperature T in units of $t=\text{bandwidth}/4$ at various couplings.

Further, the calculated phonon probability distribution $P(x)$ (not shown) reveals that the double-well form discussed by Yu and Anderson occurs only in the low T , large g 'insulating' regime. Thus anharmonicity, while quantitatively important, is not the fundamental cause of the phenomenon.

The remaining issue is assumption (2): the relation of the self-energy to the scattering mechanism. The weak-coupling (Migdal) result for our model is $\Sigma''(\omega = 0) = g^2 \langle x^2 \rangle (1 - (\mu/2t)^2)^{1/2}$. To see how this relationship evolves we plot in Fig 4 $\Sigma''(\omega = 0)/g^2 \langle x^2 \rangle$ as a function of temperature at different couplings.

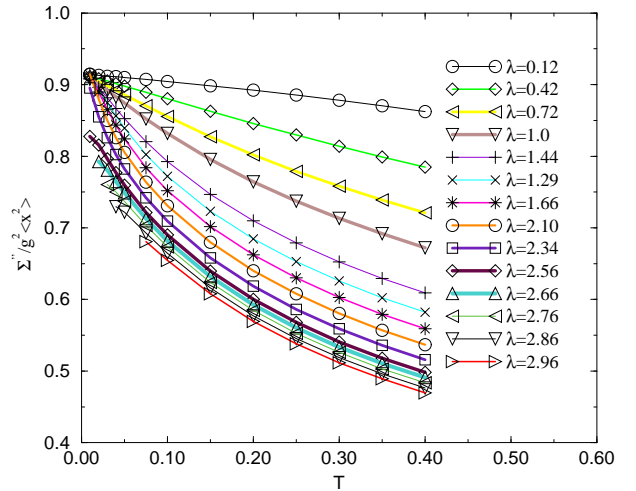


Fig 4 $\Sigma''(\omega = 0)/g^2 \langle x^2 \rangle$ vs. temperature T at various

couplings.

We see that as $g^2 < x^2 >$ increases, the ratio falls sharply below the weak coupling value and indeed ultimately $\Sigma''(\omega = 0)$ becomes proportional to $(g^2 < x^2 >)^{1/2}$ i.e. roughly to $T^{1/2}$. The crossover may be understood analytically from Eq 3. At low T and small $g, a \sim it$ so one may expand in gx/a , generating the familiar Migdal series. At high T and large g a is negligible and the integral is dominated by a pole at $x \sim it/g$; taking account of the normalization of $P(x)$ yields $G_{loc} \sim 1/g \langle x^2 \rangle^{1/2}$ and so $\Sigma \sim g \langle x^2 \rangle^{1/2}$. *Thus the key to saturation is that at strong coupling the scattering rate continues to increase but at a rate less rapid than that given by second order perturbation theory.* A similar result for the self energy of a model of carriers coupled to spin fluctuations was presented in [15].

We now add disorder scattering. Qualitatively one may think of impurities as adding an extra T -independent term to $\langle x^2 \rangle$, so $\langle x^2 \rangle \rightarrow \langle x_{phonon}^2(T) + x_{impurity}^2 \rangle$. At low T and small λ the rates add, leading to Matthiessen's rule $\rho = \rho_{phonon} + \rho_{impurity}$. At high T , physical quantities depend on $\langle x^2 \rangle^{1/2}$ so the relative correction due to impurities is of order $x_{impurity}^2/x_{phonon}^2(T)$: Matthiessen's rule does not apply. Fig 5 shows the results of a direct calculation confirming this idea. A more sophisticated (non-CPA) treatment is required to reproduce the observed negative $d\rho/dT$ at very strong disorder.

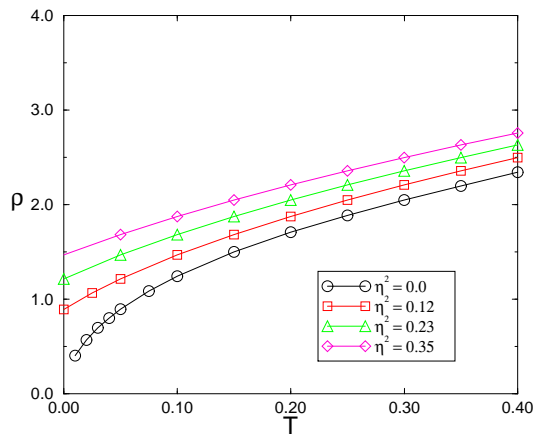


Fig 5 Impurity dependence of resistivity; $\lambda = 2.34$, $n=1/2$.

To summarize, we have shown that a simple model of electrons coupled to classical phonons and to static disorder reproduces very well the essential features of the phenomenon usually described as resistivity saturation. The cause of the phenomenon was found to be a breakdown of the Migdal relation between lattice distortion amplitude and electron self energy. Comparison of our results for different carrier densities along with the band-mixing arguments of Ref [8], indicates that the value of A/B will depend strongly on model details, so detailed compari-

son of our calculation to experiments on specific materials is inappropriate, but material-specific calculations using the ideas and formalism put forward here would be of great interest.

Our results imply that the term 'saturation' is a misnomer: there is no intrinsic maximum value of the high-temperature resistivity. Indeed at very high temperatures one expects classical diffusion with diffusion constant D vanishing or tending to a constant as $T \rightarrow \infty$, implying ρ increasing indefinitely with T . This was found in 'retracable path approximation' studies of the Hubbard model [16] and recently in a model of carriers coupled to magnetically correlated spins [17]. From this perspective the 'absence of saturation' [7] in correlated electron materials is not by itself surprising; the interesting issue is the apparent smoothness of the crossover from the low- T coherent transport regime to the high- T classical diffusion regime.

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- [1] N. W. Ashcroft and N. D. Mermin *Solid State Physics* (Holt, Rinehart and Wilson, New York: 1976), ch. 26.
 - [2] Z. Fisk and G. W. Webb, Phys. Rev. Lett. **36** 1084 (1976).
 - [3] H. Lutz et. al., Phys. Rev. Lett. **36** 1576 (1976); see also Z. Fisk and A. G. Lawson, Sol. St. Comm. **13** 277 (1973) and J. H. Mooij, Phys. Status Solidi **A17** 521 (1973).
 - [4] M. Gurvitch and A. T. Fiory, Phys. Rev. Lett. **59** 1337 (1987)
 - [5] A. F. Hebard et. al., Phys. Rev. **B48** 9945 (1993).
 - [6] L. Klein et. al., Phys. Rev. Lett. **77** 2774 (1996).
 - [7] V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74** 3253 (1995).
 - [8] B. Chakraborty and P. B. Allen, Phys. Rev. Lett. **42** 736 (1979) and Phys. Rev. **B23** 4815 (1981).
 - [9] D. Belitz and W. Schirmacher, J. Phys. **C16** 913 (1983).
 - [10] M. Gurvitch in *Superconductivity in d and f band metals*, H. Suhl and M. B. Maple, eds (New York: 1980) p. 317.
 - [11] C.C. Yu and P. W. Anderson, Phys. Rev. **B29** 6165 (1984).
 - [12] A. B. Migdal, Sov. Phys. J.E.T.P. **7** 996 (1958).
 - [13] A. Georges et. al. Rev. Mod. Phys. **68**, 13 (1996)
 - [14] A. J. Millis et. al., Phys. Rev. B **54**, 5389 (1996).
 - [15] A. V. Chubukov and D. Morr, (cond-mat/9806200)
 - [16] W. F. Brinkman and T. M. Rice, Phys. Rev. **B2** 1324 (1970).
 - [17] A. Parcollet and A. Georges, (cond-mat/9806119).